

quantum mechanicsPavel Kundrát ^{*}, Miloš Lokajíček [†]*Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2,**CZ-182 21 Praha 8, Czech Republic***Abstract**

The problem of defining time (or phase) operator for three-dimensional harmonic oscillator has been analyzed. A new formula for this operator has been derived. The results have been used to demonstrate a possibility of representing quantum-mechanical time evolution in the framework of an extended Hilbert space structure. Physical interpretation of the extended structure has been discussed shortly, too.

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^{*}E-mail: Pavel.Kundrat@fzu.cz

[†]E-mail: lokaj@fzu.cz

I. INTRODUCTION

The description of time evolution in the framework of the standard quantum mechanics represents a problem that has not yet been satisfactorily solved, even if the given theory is based in principle on the time-dependent Schrödinger equation. The first attempt of defining an operator, the expectation values of which corresponded to increasing time, was undertaken by Dirac [1] already in 1927. He tried to express the operator fulfilling the condition

$$i[H, T] = 1 \quad (1)$$

for linear harmonic oscillator (or electromagnetic field) with the help of annihilation and creation operators. He defined the operator

$$\mathcal{E} = \exp(-i\omega T) \quad (2)$$

fulfilling corresponding commutation relations with Hamiltonian

$$[H, \mathcal{E}] = -\omega\mathcal{E}, \quad [H, \mathcal{E}^\dagger] = \omega\mathcal{E}^\dagger. \quad (3)$$

However, it was shown later by Susskind and Glogover [2] that the required unitarity of this operator did not hold for all states of the standard Hilbert space, as $\mathcal{E}^\dagger\mathcal{E}|0\rangle = 0$; i.e., the condition has not been fulfilled for the state of minimum energy (vacuum state). Many authors have tried to remove this difficulty and to find a suitable modification of the standard Hilbert space enabling to define a unitary phase exponential operator \mathcal{E} ; see, e.g., the review of Lynch [3].

The situation has been complicated due to the other argument presented by Pauli [4] already in 1933. He showed that the existence of time operator T fulfilling Eq. (1) in the standard Hilbert space (i.e., in the Hilbert space spanned on a simple basis of Hamiltonian eigenvectors) required for Hamiltonian H to possess continuous energy spectrum from the whole interval $E \in (-\infty, +\infty)$, which contradicts the energy non-negativity (or at least energy limited from below).

It has been generally assumed that both these problems have followed from one common source and may be solved with the help of one approach. However, in fact they represent two different problems, which may manifest better in the three-dimensional case than in the linear one.

In Sec. II we will repeat shortly the problem concerning the case of linear harmonic oscillator; some approaches trying to solve the question of non-unitarity of exponential phase operator will be mentioned, too. The time (phase) operator for a three-dimensional harmonic oscillator will be derived newly in Sec. III. In Sec. IV the doubled Hilbert space will be constructed for this system, using the approach of Fain [5] and Newton [6]. This approach has been originally proposed for removing the problem in the case of linear harmonic oscillator; however, the physical meaning of the enlarged Hilbert space may be followed better in the three-dimensional case. The objection of Pauli may be then removed with the help of a construction corresponding to the approach of Lax and Phillips [7], which is described in Sec. V. It allows to represent individual time-dependent solutions of Schrödinger equation by corresponding trajectories in suitably extended Hilbert space. Thus, the problems concerning the time operator in quantum mechanics may be solved completely with the help of suitable Hilbert space modification. The possible physical interpretation of this modification will be then mentioned in concluding Sec. VI.

II. LINEAR HARMONIC OSCILLATOR

In trying to define the time operator in the case of linear harmonic oscillator Dirac [1] started from the relation fulfilled by annihilation and creation operators

$$[H, a] = -\omega a, \quad [H, a^\dagger] = \omega a^\dagger. \quad (4)$$

It was possible to define operators

$$\mathcal{E} = (a^\dagger a + 1)^{-1/2} a, \quad \mathcal{E}^\dagger = a^\dagger (a^\dagger a + 1)^{-1/2}, \quad (5)$$

fulfilling commutation relations (3) and corresponding to Eq. (2). The operators \mathcal{E} and \mathcal{E}^\dagger should be, therefore, unitary. However, as already mentioned it was shown by Susskind and Glogower [2] that it held

$$\mathcal{E}\mathcal{E}^\dagger = 1, \quad \mathcal{E}^\dagger\mathcal{E} = 1 - |0\rangle\langle 0|; \quad (6)$$

$|0\rangle\langle 0|$ being the projector onto the vacuum state. It means that the given operators have been isometric only, but not unitary in the standard Hilbert space; they have not represented, therefore, a full quantum-mechanical analogue of the classical phase exponential.

The action of \mathcal{E} on the number-state vector basis $\{|n\rangle\}$ reads

$$\begin{aligned} \mathcal{E} |n > 0\rangle &= |n - 1\rangle, \\ \mathcal{E} |n = 0\rangle &= 0, \\ \mathcal{E}^\dagger |n\rangle &= |n + 1\rangle, \end{aligned} \quad (7)$$

which can be illustrated by the following scheme:

$$0 \leftarrow |0\rangle \rightleftharpoons |1\rangle \rightleftharpoons |2\rangle \rightleftharpoons \dots, \quad (8)$$

where \mathcal{E} shifts to the left and \mathcal{E}^\dagger to the right.

The non-unitarity of the shift operators \mathcal{E} , \mathcal{E}^\dagger has related to semi-boundedness of the Hamiltonian spectrum. However, it has not been clear what is the relation to the criticism of Pauli [4] that should be considered more serious. It has not been clear, either, what role has been played by the fact that until now the problem has been discussed in the framework of one-dimensional system only. However, before discussing the three-dimensional system, let us mention several approaches used to define unitary phase exponential operator for the linear harmonic oscillator.

A review of the problem, including many theoretical approaches used so far and brief survey of experimental studies, was published by Lynch [3]. Actual solution of the problem lies in introducing a modified (extended) Hilbert space. Fain [5] and later independently Newton [6] studied an enlarged (doubled) Hilbert space consisting of two mutually orthogonal copies of the standard space,

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \quad (9)$$

with the basis $\{|n, \pm\rangle\}$. Such a structure allows a unitary phase (or time) exponential operator $\mathcal{E} = e^{i\Phi}$ to exist if this operator mutually links the vacuum states of both the subspaces:

$$\mathcal{E} = \sum_{n=0}^{\infty} |n, +\rangle \langle n+1, +| + |0, -\rangle \langle 0, +| + \sum_{n=0}^{\infty} |n+1, -\rangle \langle n, -|. \quad (10)$$

Its action on the basis chain can be depicted by the scheme

$$\dots \Rightarrow |2, -\rangle \Rightarrow |1, -\rangle \Rightarrow |0, -\rangle \Rightarrow |0, +\rangle \Rightarrow |1, +\rangle \Rightarrow |2, +\rangle \Rightarrow \dots, \quad (11)$$

where \mathcal{E} shifts to the left and \mathcal{E}^\dagger to the right.

As to the physical meaning of the doubled Hilbert space, Newton has admitted two possible ways of Hilbert space modification, the pseudo-spin and negative-number-state extensions [8] of the standard Hilbert space, differing by the sign of Hamiltonian on the subspace \mathcal{H}_- . However, he has considered the subspace \mathcal{H}_- to be merely auxiliary, the physical meaning being ascribed to the projection onto the subspace \mathcal{H}_+ only. On the other hand, Fain has interpreted the doubled Hilbert space in analogy to classical mechanics; the two subspaces have corresponded to two possible ways of connecting phase and time, $\varphi = \varphi_0 + \omega t$ or $\varphi = \varphi_0 - \omega t$.

Modifications of the Hilbert space proposed by other authors seem to be more complicated. E.g., Pegg and Barnett [9] have considered a series of finite-dimensional Hilbert spaces \mathcal{H}_s where the phase exponential operator with the finite basis chain $\{|n\rangle\}_{n=0}^s$ have formed a cyclic group; the dimension $(s+1)$ of the space has been allowed to tend to infinity after physical results (expectation values) have been calculated in the finite-dimensional space \mathcal{H}_s . Ban [10] and similarly Luis and Sánchez-Soto [11] have tried to solve the quantum phase problem by studying the phase-difference operator between two systems. Another attempt to solve the given problem has been made, e.g., by Vaccaro [12]. An extended Hilbert space structure has been used also by Ozawa [13]. A more systematic approach has been proposed by Yu and Zhang [14]. However, the proposals of Fain or Newton seem to have

been the most simple and to represent a natural way of removing the non-unitarity of phase exponential operator.

III. THREE-DIMENSIONAL HARMONIC OSCILLATOR

We will derive now the exponential phase operator for three-dimensional harmonic oscillator, which is being applied to in many physical processes, e.g., in nuclear physics. The Hamiltonian for such an oscillator may be written as

$$H = \frac{(\mathbf{p})^2}{2M} + \frac{1}{2}k(\mathbf{r})^2, \quad (12)$$

where \mathbf{r} , \mathbf{p} are position and momentum vectors, M mass of the particle, $\omega = \sqrt{\frac{k}{M}}$ angular frequency.

It is then possible to introduce vector operators

$$\mathbf{Y} = \mathbf{p} - iM\omega\mathbf{r}, \quad \mathbf{Y}^\dagger = \mathbf{p} + iM\omega\mathbf{r}, \quad (13)$$

that satisfy commutation relations

$$[H, Y_j] = -\omega Y_j, \quad [H, Y_j^\dagger] = \omega Y_j^\dagger. \quad (14)$$

It holds also

$$[H, Y^2] = -2\omega Y^2, \quad [H, (Y^2)^\dagger] = 2\omega (Y^2)^\dagger, \quad (15)$$

where $Y^2 = \mathbf{Y} \cdot \mathbf{Y}$, $(Y^2)^\dagger = \mathbf{Y}^\dagger \cdot \mathbf{Y}^\dagger$.

The angular momentum $L_k = \varepsilon_{ijk} r_i p_j$, $L^2 = \sum_k L_k^2$ fulfils commutation relations

$$[H, L_k] = 0, \quad [H, L^2] = 0. \quad (16)$$

It holds also

$$[L_k, Y_l] = i\varepsilon_{klm} Y_m, \quad [L_k, Y^2] = 0; \quad (17)$$

operator Y^2 does not mix different partial waves.

It is then possible to introduce operators Z and Z^\dagger :

$$\begin{aligned} Z &= \frac{1}{2M} \left[(H + \omega)^2 - \omega^2 \left(L^2 + \frac{1}{4} \right) \right]^{-1/2} Y^2, \\ Z^\dagger &= (Y^2)^\dagger \frac{1}{2M} \left[(H + \omega)^2 - \omega^2 \left(L^2 + \frac{1}{4} \right) \right]^{-1/2}, \end{aligned} \quad (18)$$

fulfilling

$$[H, Z] = -2\omega Z, \quad [H, Z^\dagger] = 2\omega Z^\dagger \quad (19)$$

and also

$$ZZ^\dagger = 1. \quad (20)$$

Operator Z acts as a shift operator (similarly as \mathcal{E} in one-dimensional case):

$$\begin{aligned} Z|n > 0, lm\rangle &= |n - 1, lm\rangle, \\ Z|0, lm\rangle &= 0, \\ Z^\dagger|nlm\rangle &= |n + 1, lm\rangle, \end{aligned} \quad (21)$$

where $|nlm\rangle$ are corresponding eigenfunctions of the Hamiltonian H , of total angular momentum L^2 , and of its component L_z :

$$\begin{aligned} H|nlm\rangle &= \omega(2n + l + 3/2)|nlm\rangle, \\ L^2|nlm\rangle &= l(l + 1)|nlm\rangle, \\ L_z|nlm\rangle &= m|nlm\rangle, \end{aligned} \quad (22)$$

where $n = 0, 1, 2, \dots$; $l = 0, 1, 2, \dots$; $m = -l, \dots, +l$. It means that the operator Z is an isometry operator; it violates the unitarity when acting on vacuum state vectors ($n = 0$), similarly as in the one-dimensional case.

IV. DOUBLED HILBERT SPACE

Similarly to the one-dimensional case, it is possible to form the doubled Hilbert space

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \quad (23)$$

consisting of two mutually orthogonal copies isomorphic to the standard Hilbert space. All operators act on both the subspaces in the same way as in the standard Hilbert space.

It is convenient to use sign operator I [5,8] distinguishing the individual subspaces, which yields the eigenvalue of $+1$ for \mathcal{H}_+ and -1 for \mathcal{H}_- , and also to introduce the exchange operator X , which interchanges the subspaces \mathcal{H}_+ and \mathcal{H}_- , leaving other characteristics of the state unchanged; it holds, e.g., $X^2 = 1$, $XI = -IX$, $XH = HX$, $XL_k = L_kX$. The sign operator I plays the role of a superselection operator, as pointed out already by Bauer [8] in the case of linear oscillator.

The phase exponential operator $\mathcal{E} = e^{i\Phi}$ may be then defined by

$$\begin{aligned} \mathcal{E}^2 &= \frac{1+I}{2} Z + \frac{1-I}{2} Z^\dagger + X (1 - Z^\dagger Z) \frac{1+I}{2}, \\ (\mathcal{E}^\dagger)^2 &= Z^\dagger \frac{1+I}{2} + Z \frac{1-I}{2} + \frac{1+I}{2} (1 - Z^\dagger Z) X, \end{aligned} \quad (24)$$

i.e., it corresponds to Z and Z^\dagger on the individual subspaces and links mutually the vacuum states of both the subspaces. The inverse formulae read

$$\begin{aligned} Z &= \frac{1+I}{2} \mathcal{E}^2 + \frac{1-I}{2} (\mathcal{E}^\dagger)^2, \\ Z^\dagger &= (\mathcal{E}^\dagger)^2 \frac{1+I}{2} + \mathcal{E}^2 \frac{1-I}{2}. \end{aligned} \quad (25)$$

The time operator may be then defined by

$$T = -\Phi/\omega. \quad (26)$$

Introducing sine and cosine operators

$$e^{\pm i\Phi} = \cos \Phi \pm i \sin \Phi, \quad (27)$$

one may write

$$\begin{aligned} (\mathbf{p} - iM\omega\mathbf{r})^2 &= 2M \left[(H + \omega)^2 - \omega^2 \left(L^2 + \frac{1}{4} \right) \right]^{1/2} (\cos 2\Phi + iI \sin 2\Phi), \\ (\mathbf{p} + iM\omega\mathbf{r})^2 &= (\cos 2\Phi - iI \sin 2\Phi) 2M \left[(H + \omega)^2 - \omega^2 \left(L^2 + \frac{1}{4} \right) \right]^{1/2}, \end{aligned} \quad (28)$$

i.e., the position and momentum may be expressed in terms of the phase.

In the standard basis of the doubled Hilbert space $\{|n, l, m; \lambda\rangle, \lambda = \pm 1\}$, the sign and exchange operators act according to

$$\begin{aligned} I|n, l, m; \lambda\rangle &= \lambda|n, l, m; \lambda\rangle, \\ X|n, l, m; \lambda\rangle &= |n, l, m; -\lambda\rangle, \end{aligned} \quad (29)$$

and the definition of the phase exponential operator reads

$$\begin{aligned} e^{2i\Phi} &= \sum_{l=0}^{\infty} \sum_{m=-l}^l \left(\sum_{n=0}^{\infty} |n, lm; +\rangle \langle n+1, lm; +| + \right. \\ &\quad \left. + |0, lm; -\rangle \langle 0, lm; +| + \sum_{n=0}^{\infty} |n+1, lm; -\rangle \langle n, lm; -| \right), \\ e^{-2i\Phi} &= \sum_{l=0}^{\infty} \sum_{m=-l}^l \left(\sum_{n=0}^{\infty} |n+1, lm; +\rangle \langle n, lm; +| + \right. \\ &\quad \left. + |0, lm; +\rangle \langle 0, lm; -| + \sum_{n=0}^{\infty} |n, lm; -\rangle \langle n+1, lm; -| \right). \end{aligned} \quad (30)$$

Let us note that the doubling procedure in the three-dimensional case concerns the radial quantum number n only, states with different l or m are not mixed together. For each l, m there is the chain similar to (11)

$$\begin{aligned} \dots &\rightleftharpoons |2, lm; -\rangle \rightleftharpoons |1, lm; -\rangle \rightleftharpoons |0, lm; -\rangle \rightleftharpoons \\ &\rightleftharpoons |0, lm; +\rangle \rightleftharpoons |1, lm; +\rangle \rightleftharpoons |2, lm; +\rangle \rightleftharpoons \dots, \end{aligned} \quad (31)$$

where the operator $e^{2i\Phi}$ shifts to the left and $e^{-2i\Phi}$ to the right.

The matrix elements of the commutator $[H, e^{\pm 2i\Phi}]$ between arbitrary states $|\chi_+\rangle, |\psi_+\rangle \in \mathcal{H}_+$ fulfil

$$\langle \chi_+ | [H, e^{\pm 2i\Phi}] | \psi_+ \rangle = \mp 2\omega \langle \chi_+ | e^{\pm 2i\Phi} | \psi_+ \rangle. \quad (32)$$

For the expectation value of $e^{\pm 2i\Phi}$ in an instantaneous state $|\psi_+(t)\rangle = e^{-iHt} |\psi_+(0)\rangle$ it holds

$$\langle \psi_+(t) | e^{\pm 2i\Phi} | \psi_+(t) \rangle = \langle \psi_+(0) | e^{\pm 2i\Phi} | \psi_+(0) \rangle e^{\mp 2i\omega t}. \quad (33)$$

For state $|\psi_-\rangle \in \mathcal{H}_-$, these relations differ by additional minus sign, leading to the expectation value of $e^{\pm 2i\Phi}$ proportional to $e^{\pm 2i\omega t}$.

V. DETAILED HILBERT SPACE STRUCTURE AND EVOLUTION OPERATOR

In the doubled Hilbert space described in the preceding section, both the subspaces have remained permanently orthogonal and separated; evolution operator $U(t) = e^{-iHt}$ acting always in one subspace. It has been possible to define the unitary phase exponential operator. However, the relation to the objection of Pauli has not been clear.

In fact, the problem of Pauli concerning a regular representation of quantum-mechanical time evolution has been solved in the scattering theory of Lax and Phillips [7,15] (for summary, see [16]). The solutions of time-dependent Schrödinger equation have been represented as trajectories in extended Hilbert space consisting of the subspace \mathcal{D}_- of incoming states and the subspace \mathcal{D}_+ of outgoing states, being connected with the help of evolution operator $U(t)$. The following conditions have been fulfilled

$$U(t)\mathcal{D}_+ \subset \mathcal{D}_+ \quad \forall t \geq 0, \quad \bigcap_{t \geq 0} U(t)\mathcal{D}_+ = 0, \quad \overline{\bigcup_{t \in R} U(t)\mathcal{D}_+} = \mathcal{H}, \quad (34)$$

$$U(t)\mathcal{D}_- \subset \mathcal{D}_- \quad \forall t \leq 0, \quad \bigcap_{t \leq 0} U(t)\mathcal{D}_- = 0, \quad \overline{\bigcup_{t \in R} U(t)\mathcal{D}_-} = \mathcal{H}. \quad (35)$$

The same structure has been derived by Alda et al. [17] for the description of a purely exponential decay of an unstable particle, the total Hilbert space being formed by the subspaces of unstable particle, of its decay products (\mathcal{D}_+), and of colliding particles (\mathcal{D}_-) producing the given unstable particle.

Let us also mention that within the theory of Lax and Phillips, the existence of a Hermitian (self-adjoint) time operator is a direct consequence of the structure of the Hilbert space, i.e., of the existence of the incoming and outgoing subspaces. Thus the Hilbert space structure of Lax and Phillips may be considered as a solution to the objection of Pauli. It enables to represent the irreversible evolution already on the level of microscopic objects. A more detailed discussion of the whole problem will be presented elsewhere [18].

A similar approach may be applied also to the case of periodic systems, e.g., to three-dimensional harmonic oscillator. The individual Fain's subspaces \mathcal{H}_+ , \mathcal{H}_- are then formed

by a series of subspaces that are mutually linked by the action of evolution operator. The total Hilbert space structure has the form of

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_- \oplus \mathcal{H}_+ , \\ \mathcal{H}_\pm &= \sum_{j=-\infty}^{\infty} \left(\mathcal{D}_{-,j}^{(\pm)} + \mathcal{D}_{+,j}^{(\pm)} \right) .\end{aligned}\tag{36}$$

The individual subspaces contain solutions of the time-dependent Schrödinger equation. E.g., the subspace $\mathcal{D}_{-,j}^{(\pm)}$ for given j is formed by all the instantaneous states belonging to the solutions of Schrödinger equation corresponding to one half of a period of evolving system. Other subspaces are generated by the action of the evolution operator according to

$$\begin{aligned}U(T_0/2) \mathcal{D}_{-,j}^{(\pm)} &= \mathcal{D}_{+,j}^{(\pm)} , \\ U(T_0/2) \mathcal{D}_{+,j}^{(\pm)} &= \mathcal{D}_{-,j+1}^{(\pm)} ;\end{aligned}\tag{37}$$

T_0 being the period of the system.

In each of the individual subspaces $\mathcal{D}_{\pm,j}^{(\pm)}$, the phase Φ is confined to a corresponding interval:

$$\begin{aligned}\mathcal{D}_{-,j}^{(+)} \quad \dots \quad &-2j\pi < \phi \leq \pi - 2j\pi , \\ \mathcal{D}_{+,j}^{(+)} \quad \dots \quad &-\pi - 2j\pi < \phi \leq -2j\pi , \\ \mathcal{D}_{-,j}^{(-)} \quad \dots \quad &-\pi + 2j\pi < \phi \leq +2j\pi , \\ \mathcal{D}_{+,j}^{(-)} \quad \dots \quad &+2j\pi < \phi \leq \pi + 2j\pi .\end{aligned}\tag{38}$$

The phase operator Φ exhibits monotonous behavior during time evolution. According to (32) - (33), the expectation value of phase $\langle \Phi \rangle$ continuously decreases with time in the subspace \mathcal{H}_+ (increases in \mathcal{H}_-); the expectation value τ of the time operator T increases or decreases in a similar way:

$$\begin{aligned}\langle \Phi \rangle(t) &= \langle \Phi \rangle(0) \mp \omega t , \\ \tau(t) &= \tau(0) \pm t .\end{aligned}\tag{39}$$

VI. CONCLUSION

Many physical problems have been demonstrated and solved often with the help of linear (one-dimensional) systems. However, in such a case actual characteristics may be simplified and some important properties of three-dimensional systems may be hidden, which has concerned also the problem of defining time operator. E.g., the full sense of Fain's proposal may be seen only in the case of the three-dimensional oscillator, as individual Hilbert subspaces seem to correspond to different orientations of the angular momentum vector. It might also indicate a way how to test experimentally the physical meaning of Fain's doubling procedure.

The given scheme has been proposed to remove the problem with the non-unitarity of phase exponential operator in the case of harmonic oscillator. Individual subspaces have remained separated during the whole time evolution. To solve the problem of Pauli, both the subspaces should be formed further by a chain of other subspaces that are mutually linked by the action of evolution operator. The resulting structure corresponds to that proposed earlier by Lax and Phillips for the description of scattering phenomena. All dynamical properties of the solutions of time-dependent Schrödinger equation may be correctly represented, and the phase and time operators may be defined regularly, which enables one to distinguish between states corresponding to different points of time evolution.

Therefore, the use of the more complex Hilbert space structure seems to be not only formal, as sometimes stated, but also physically reasonable and practically necessary. The use of the structure described in the preceding enables us to represent the time evolution of periodic and non-periodic systems on the similar basis.

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